

Short-coherence length superconductivity in the Attractive Hubbard Model in three dimensions

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We study the normal state and the superconducting transition in the Attractive Hubbard Model in three dimensions, using self-consistent diagrammatics. Our results for the self-consistent T -matrix approximation are consistent with 3D-XY power-law critical scaling and finite-size scaling. This is in contrast to the exponential 2D-XY scaling the method was able to capture in our previous 2D calculation. We find the 3D transition temperature at quarter-filling and $U = -4t$ to be $T_c = 0.207t$. The 3D critical regime is much narrower than in 2D and the ratio of the mean-field transition to T_c is about 5 times smaller than in 2D. We also find that, for the parameters we consider, the pseudogap regime in 3D (as in 2D) coincides with the critical scaling regime.

Inspired by the discovery of high-temperature superconductors there has been considerable interest for some time in understanding how the BCS picture gets modified in the case of short coherence length superconductivity. A simple model for a correlated superconductor is the Attractive Hubbard Model that allows one to tune the attraction to an intermediate regime between the BCS and Bose limits [1] where the fermions are still degenerate but the coherence length starts to approach the interparticle spacing. Earlier studies [2] of this model in 2D using Monte Carlo methods revealed the development of a pseudogap in the normal state. In this paper we employ self-consistent diagrammatics that is a variant of the Fluctuation-Exchange Approximation [3–6]. Specifically, we use the self-consistent T -matrix approximation (STA) that only retains fluctuations in the particle-particle channel. These are presumably the only relevant fluctuations in the model for the densities we consider. We have found before [7] that quite remarkably, the STA approach in 2D captures the critical 2D-XY fluctuations with a Kosterlitz-Thouless (KT) transition temperature in good agreement with Monte Carlo [8]. In addition we found a very broad critical regime that coincides with the development of a normal state pseudogap. It is very surprising that self-consistent diagrammatics can capture critical behaviour relatively well. In order to understand this better, and encouraged by the success in 2D, we now study this model in three dimensions where techniques like Monte Carlo are severely limited by system size constraints.

We find that the STA method indeed yields results in three dimensions that are consistent with the expected power-law scaling rather than the exponential KT-scaling we found in 2D. In addition, the success of finite-size scaling allows us to determine T_c in 3D. In addition to observing a much narrower pseudogap regime than in 2D, we can quantify the difference in pairbreaking fluctuations by looking at the ratio of the mean-field (1-loop) T_c to the actual transition temperature and find that this ratio drops from 12 to about 2.6 in going from 2D to 3D, for the parameters we consider. We also conclude that since the dramatic KT-scaling observed in 2D is not seen in

3D, this result is not a numerical artifact.

While superconductivity in the Attractive Hubbard Model is of course s -wave, it is fair to assume that the strong correlation effects in this model will also apply to a more realistic d -wave theory. In fact, an advantage of the STA is that one can explicitly consider models with d -wave attraction [9]. In the context of the cuprates our work suggests that the loss of low-energy spectral weight in the pseudogap normal state can be attributed to pre-cursor pairing as observed in our calculation. By studying dimensionality, the observation then is that underdoped cuprates behave more like our 2D calculations while optimally and overdoped materials have pseudogap behaviour more in line with our 3D results. Since, within a given family of materials, the anisotropy can increase several hundred-fold upon underdoping, the implication is that this change in effective dimensionality plays an important role in enhancing the underdoped pseudogap.

Our starting point is the hamiltonian for the Attractive Hubbard Model

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + hc - |U| \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where the tight-binding hopping sums over nearest neighbour pairs on a three-dimensional square lattice and the potential captures singlet pairing for a short-range potential. The standard perturbative approach is to evaluate the pair susceptibility at the 1-loop level. Such a Gaussian theory amounts to re-summing the BCS ladder diagrams yielding an RPA-like form

$$\chi_{\text{gaus}}(\mathbf{q}, i\omega_n) = \frac{\Pi_0(\mathbf{q}, i\omega_n)}{1 - |U| \Pi_0(\mathbf{q}, i\omega_n)} \quad (2)$$

where $i\omega_n$ are Matsubara frequencies and Π_0 is the bare bubble in terms of free fermion propagators. In the limit of small U , this framework reduces to BCS-theory. We are interested in intermediate attraction where the fermions are still degenerate but the pairing is strong. The value $U = -4t$ that we use throughout this paper is representative of such intermediate attraction. The model also deviates strongly from BCS theory near half-filling, where the Attractive Hubbard Model maps into

the Hubbard Model with on-site repulsion. Since we do not wish to include the effects of the associated CDW instability at half-filling, all our results in this paper will focus on quarter-filling.

The superconducting instability signaled by the Thouless criterion that determines the transition temperature as the highest temperature that satisfies $1/\chi_{\text{gaus}}(T = T_c) = 0$.

Our approach is to extend this framework to the self-consistent T -matrix (STA) formulation, which simply generalises the bare bubble in (2) with dressed propagators for the intermediate fermion states:

$$\Pi(\mathbf{q}, i\omega_n) = \frac{-1}{\beta} \sum_{\mathbf{k}, ik_n} G(\mathbf{q}-\mathbf{k}, i\omega_n - ik_n) G(\mathbf{k}, ik_n) \quad (3)$$

where the dressed Green's function $G(\mathbf{k}, ik_n) = [ik_n - \epsilon_{\mathbf{k}} + \mu - \Sigma(\mathbf{k}, ik_n)]^{-1}$ is defined in terms of the pair susceptibility itself, through the self-energy:

$$\Sigma(\mathbf{k}, ik_n) = \frac{1}{\beta} \sum_{\mathbf{q}, i\omega_n} G(\mathbf{q}-\mathbf{k}, i\omega_n - ik_n) \Gamma(\mathbf{q}, i\omega_n). \quad (4)$$

Technically, we explicitly keep only corrections of order U^2 and higher which implies that the Hartree term is already included in the unperturbed chemical potential. This higher order contribution is expressed through the effective interaction:

$$\Gamma(\mathbf{q}, i\omega_n) = \frac{U^2 \Pi(\mathbf{q}, i\omega_n)}{1 - |U| \Pi(\mathbf{q}, i\omega_n)}. \quad (5)$$

The self-consistent solution of equations (3) and (4) are achieved numerically, by considering a finite $N \times N \times N$ lattice with discrete momenta and only retaining a finite number of Matsubara frequencies [10]. We start off with the unperturbed solution and iteratively solve these equations (which are convolutions) using FFT's until self-consistent convergence is established.

Perturbatively this of course amounts to re-summing an infinite series of diagrams. At first one may expect that the self-consistent feedback will broaden the intermediate fermion states in (3) and simply re-scale values for physical quantities resulting from a 1-loop calculation. This is in fact not the case as can be seen from the results in Fig. 1 for the inverse of the uniform static pair susceptibility $\chi(q=0, i\omega_n=0)$ evaluated for quarter-filling $\langle n_{i\sigma} \rangle = \frac{1}{4}$ and the intermediate attraction $U = -4t$. The results are for a $32 \times 32 \times 32$ lattice. On the RHS the 1-loop result intersects the axis at $T_c^{\text{gaus}}(3D) = 0.532t$. This result is essentially independent of lattice size and the 1-loop approximation yields a non-zero transition temperature even for finite systems. In any exact treatment, one of course only expects phase transitions in the thermodynamic limit. We also indicate the 2D transition temperature in this 1-loop approximation for the same parameters at $T_c^{\text{gaus}}(2D) = 0.611t$.

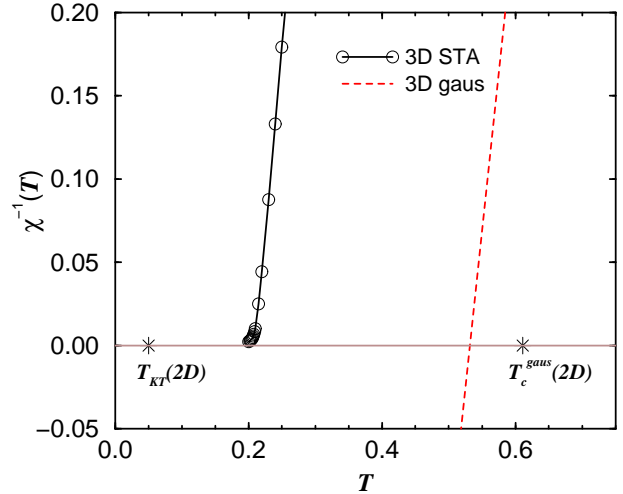


FIG. 1. Inverse pair susceptibility for a 3D lattice of linear length $L = 32$, density $\langle n_{i\sigma} \rangle = \frac{1}{4}$ and $U = -4t$. The symbols indicate the STA results and the broken line on the right is for the 1-loop (mean-field) theory. Also shown are the 2D mean-field and KT transition temperatures.

The 3D STA results indicated by the circles show a fundamentally different behaviour. The results for the inverse susceptibility never cross zero – indicating that the self-consistent calculation reflects the fact that there is no transition for a finite system. This is of course what one would expect from an exact treatment - but is missed by 1-loop theory. Simply put, the self-energy corrections sufficiently broaden the intermediate fermion propagators to avoid the superconducting instability. Thus the STA is fundamentally superior to 1-loop in that it captures the physical requirement that there are no phase transitions in finite systems.

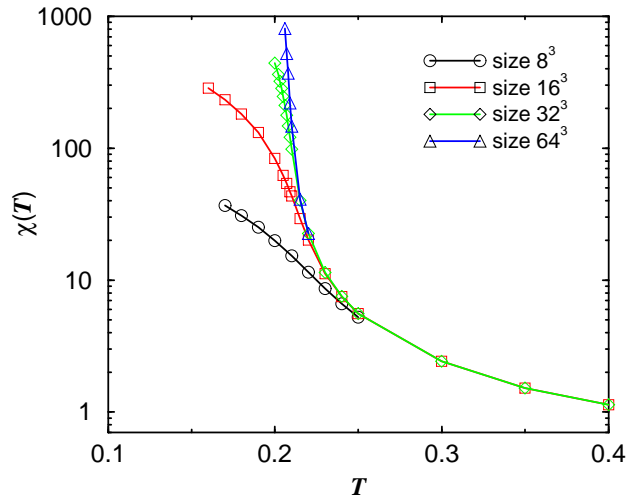


FIG. 2. Finite-size dependence of $\chi(T, L)$ in 3D for $\langle n_{i\sigma} \rangle = \frac{1}{4}$ and $U = -4t$.

Is there any more to this result? Further investigation reveals that the low-temperature static uniform pair sus-

ceptibility $\chi(T, L)$ for the STA depends on system size as shown in Fig. 2. Just as one would expect from fundamental principles, the susceptibility increases towards a maximum that is controlled by system size and can only diverge in the thermodynamic limit. Since the formalism does not include anomalous propagators, it is limited to the disordered side of the phase diagram. This plot is quite similar to our earlier results [7] in 2D, except that the attempt at a transition appears sharper and is at a higher temperature in 3D.

From this finite-size data we use standard scaling arguments [11] to extract the transition temperature in 3D. For a finite system there are two length scales namely the correlation length ξ and the system size L . One expects from a 3D scaling hypothesis that $\chi(T, L) = |T - T_c|^{-\gamma} f_1(L/\xi(T))$ where $\xi(T)$ is the correlation length in an infinite system. From $\xi(T) \sim |T - T_c|^{-\nu}$ and the scaling law $\gamma = \nu(2 - \eta)$, it follows that the following product is only a function of the ratio of the two length scales:

$$\left(\frac{1}{L}\right)^{2-\eta} \chi(T, L) = f(L/\xi(T)). \quad (6)$$

At T_c the correlation length diverges and the argument on the RHS becomes zero, independent of system size. Plots for this function for our STA data on different system sizes are given in Fig. 3. The numerical data is consistent with the finite-size scaling hypothesis and we can estimate $T_c = 0.207t$ for our standard set of parameters. This value of T is indicated by the vertical line where the plots become independent of L .

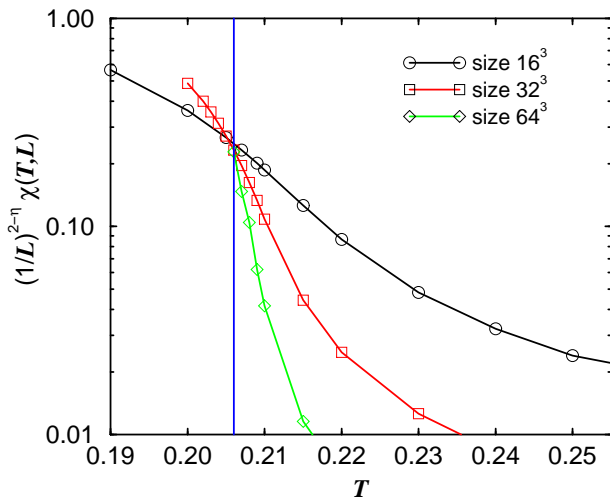


FIG. 3. Finite-size scaling of $f(L/\xi(T))$ in 3D for $\langle n_{i\sigma} \rangle = \frac{1}{4}$ and $U = -4t$. The common intersection yields $T_c = 0.207t$.

In our earlier 2D calculation, the STA yielded results that were very consistent with the Kosterlitz-Thouless scaling of the 2D-XY model, with an estimate of $T_{KT} = 0.05t$ in good agreement with previous Monte Carlo estimates [8]. In addition, we found very broad critical

scaling regime that coincides with the regime in which a pseudogap develops in the density of states at the Fermi level, $N_0(T)$. We also found very good finite-size scaling in our data. Given the difficulty of theoretically capturing the correct critical behaviour this was very surprising but one could always question whether this result was a numerical artifact.

Here we have demonstrated, that in 3D the STA data is again consistent with a finite-size scaling hypothesis – yielding the first estimate of $T_c = 0.207t$ for the parameters in question, in a calculation that goes beyond the mean-field or 1-loop class of approaches.

It is interesting to note that while the 1-loop estimate for the transition temperature is higher in 2D than in 3D for the same parameters (due to density of states effects) the opposite holds for the actual transition temperatures. We conclude that the enhanced fluctuations in 2D overcome the density of states effect. If we consider the ratio of mean-field to actual transition temperatures $R = T_c^{gaur}/T_c$ we find $R_{2D} = 0.611/0.05 \sim 12$ vs. $R_{3D} = 0.532/0.207 \sim 2.6$.

Let us next consider the bulk scaling behaviour. Is this consistent with the expected 3D-XY result

$$\chi(T) \sim \frac{1}{|T - T_c|^\gamma} \quad (7)$$

with $\gamma \simeq 1.33$? In 3D we are limited to smaller systems than in 2D and the transition itself is narrower. This limits the accuracy with which we can determine the critical scaling in the thermodynamic limit within our calculations. In Fig. 4 we plot the finite-size data $\chi(T, L)$ against the RHS of (7).

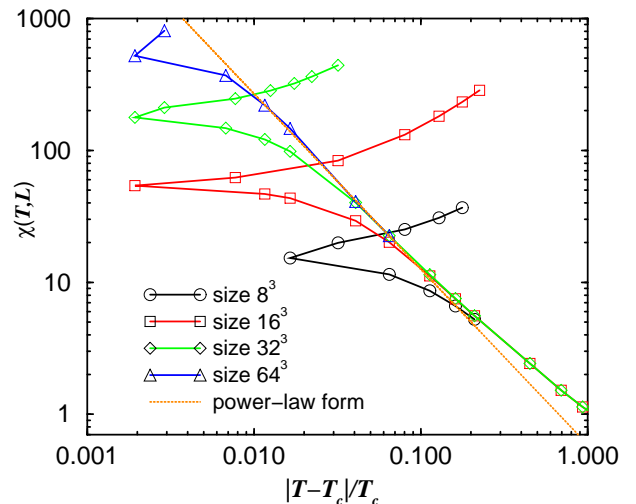


FIG. 4. Finite-size results for $\chi(T, L)$ and the expected scaling form in (7) with exponent $\gamma \simeq 1.33$.

For each system size, the high-temperature data coincides with the scaling form in (7) and at lower temperature one observes the expected finite-size corrections. While the data is clearly consistent with power-law scaling and the fit with the exponent $\gamma \simeq 1.33$ does better than the mean-

field $\gamma_{MF} = 1$, our accuracy is insufficient to determine the exponent a-priori. In addition we can estimate the width of the critical regime as extending about $0.1t$ above T_c , where the high-temperature results start to deviate from the asymptotic form.

While we cannot determine the power-law exponent, the 3D data is dramatically different from our previous 2D result that found data consistent with the exponential KT scaling expected in 2D. This gives some confidence that the 2D result was real and that the STA method captures the expected critical behaviour in both 2D and 3D quite well. This implies that for this particular model, self-consistency introduces scaling corrections that go beyond dimensional analysis – a feat that normally requires a technique such as the renormalization group. We believe that this may be connected to the rather simple $U(1)$ symmetry that superconductivity breaks, and that this result does not apply to more complicated problems.

Let us finally turn to the normal state pseudogap. The density of single-electron states can be obtained from the Green's functions dressed with our calculated self-energy corrections $\Sigma(\mathbf{k}, ik_n)$ and continued to retarded frequencies using Padé analytic continuation. In Fig. 5 we show the temperature-dependence of the density of states at the Fermi level for our standard density and interaction strength. We show results for both 3D and 2D and indicate the respective T_c 's by the vertical lines. One can clearly see that the 3D pseudogap is significantly smaller than in 2D and again coincides with the critical regime. In earlier analytic work [12], we calculated the 3D pseudogap for a continuum model within the 1-loop theory and found that even at this level, the pseudogap corrections go beyond the expected results in a small energy, long-wavelength expansion.

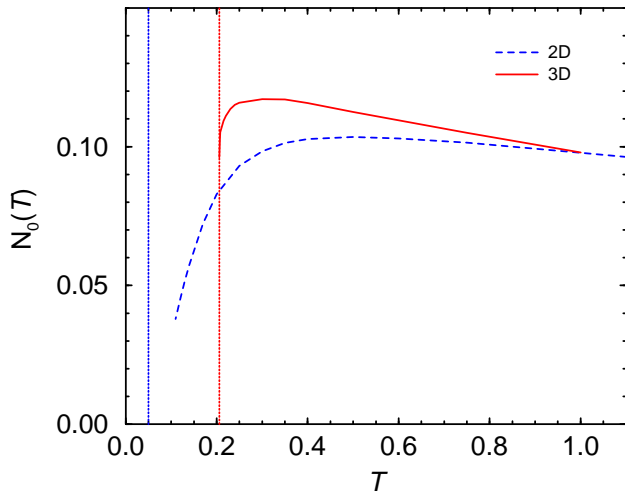


FIG. 5. Pseudogap in the density of states at the Fermi level in 3D and in 2D for $\langle n_{i\sigma} \rangle = \frac{1}{4}$ and $U = -4t$.

In summary, we have shown that results for the self-consistent T -matrix approximation in 3D are consistent with the expected finite-size and power-law critical be-

haviour for the 3D-XY model. At quarter-filling and for and intermediate attraction $U = -4t$, we find in 3D $T_c \simeq 0.207t$, about 2.6 times smaller than the mean-field transition temperature, and a narrow critical and pseudogap regime. We also find that while the mean-field transition temperature is higher in 2D than in 3D, the opposite holds for the actual T_c . Our results suggest that the previous 2D results are not a numerical artifact and that the STA formalism can distinguish between the fundamentally different nature of fluctuations in two and three dimensions.

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